

How two spins can thermalize a third spin

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We consider thermalization of a microscopic quantum system by interaction with a thermal bath. Our interest is the minimal size the bath can have while still being able to thermalize the system. Within a specific thermalization scheme we show that a single spin-1/2 can be fully thermalized by interaction with a bath that consists of just two other spin-1/2. The two bath spins are initially in a pure, entangled state, and the thermalizing interaction is a Heisenberg exchange-interaction of the system-spin with one of the bath spins. The time dependent coupling strength has to obey a single integral constraint. We also present a simple generalization of this minimal model in which the bath consists of an arbitrary number of spin-1/2 pairs.

Our topic is thermalization of a system by means of an interaction with a bath, as specified in detail below. A bath that is suitable for that purpose has to exhibit certain features. Particularly, the standard textbook discussion explicitly or tacitly assumes that some kind of thermodynamic limit regarding the bath has to be taken in order to guarantee perfect thermalization of the system. The bath is assumed to be *macroscopic* in a certain sense, also if the system to be thermalized is a microscopic one.

The purpose of this brief note is to challenge the view that the bath should always be a macroscopic one. To this end we present a simple quantum-mechanical model in which the system is a single spin-1/2, and the bath consists of only two other spin-1/2. Initially, the two bath spins are in an entangled, pure state. The system spin is shown to perfectly thermalize by means of a finite-time exchange interaction with one of the bath spins. As will be shown below, the mechanism at work is essentially swapping the states of system spin and one bath spin by the exchange interaction. As a result, the entangled initial state of the two bath spins becomes the final entangled state of the system spin and the second bath spin. Tracing out the bath spin yields the final thermal state of the system. This mechanism is neither new nor particularly intriguing. However, to the best of our knowledge, it has not yet been discussed in the context of thermalization. Doing so may help to gain further insights in this problem: as simple as our model is, it very clearly points out the important role entanglement can play in the thermalization of a system. We note that this aspect is crucial in modern theoretical approaches to the phenomenon of thermalization in general [1].

We will discuss *thermalization by a bath* within the following general scheme. A closed quantum system A , the *system*, is initially prepared in an arbitrary state associated with a density operator ρ_A . Aside A there is another closed quantum system, the *bath* B . Irrespective of the system's state ρ_A , initially the bath is always in a certain state associated with a density operator ρ_B . The third ingredient of the scheme is a time dependent interaction that is supposed to establish thermal contact between system A and bath B during a finite period of time $[0, T]$. Particularly, this means that the interaction

vanishes for $t < 0$ and $t > T$. By the interaction and the internal dynamics of A and B , the initial state $\rho_A \otimes \rho_B$ of the joint system at time $t = 0$ evolves to a final joint state ρ'_{AB} at time $t = T$. We say that the scheme thermalizes system A at some temperature β^{-1} , if for any initial state ρ_A of A the final reduced state of A ,

$$\rho'_A = \text{tr}_B \rho'_{AB},$$

is the thermal state $\tau = e^{-\beta H_A}/Z$ of the canonical ensemble. Here, H_A is the Hamiltonian of system A and $Z = \text{tr} e^{-\beta H_A}$ is its partition sum.

The above scheme is idealistic as it requires the system to be fully thermalized after an interaction during a finite period of time, $[0, T]$. To obtain a more realistic scheme one could demand that ρ'_A reaches the thermal state τ within some meaningful approximation, if necessary, for $T \rightarrow \infty$. Here we stay with the idealized scheme simply because our model meets its stronger conditions.

Admittedly, our scheme uses the notion *bath* in a loose way. For instance, it is not required that the bath itself is in some thermal equilibrium, we do not demand that it is able to thermalize an entire class of (microscopic) systems, and we also do not insist that the bath is suitable for thermalizing the system by an entire class of system-bath interactions. Significantly strengthening the scheme in this point will probably make it impossible to construct a microscopic bath. On the other hand, we think that the presented scheme still captures essential features of a general thermalization process.

It is instructive to view the thermalization of system A formally as a (rather simple) quantum operation \mathcal{T} that maps an arbitrary initial state ρ_A onto the thermal state τ . Being a proper quantum operation [2, 3], \mathcal{T} can be represented by an isometry $V : \mathcal{H}_A \rightarrow \mathcal{H}_A \otimes \mathcal{H}_B$ that is followed by taking the partial trace with respect to \mathcal{H}_B , i.e. $\mathcal{T}(\rho_A) = \text{tr}_B V \rho_A V^\dagger$ [4, 5]. Here, \mathcal{H}_A denotes the Hilbert space of system A , and \mathcal{H}_B is some appropriate ancilla Hilbert space. Since \mathcal{T} describes thermalization into τ , we have

$$\text{tr}_B V \rho_A V^\dagger = \tau \quad (1)$$

for any initial state ρ_A . This relation can be phrased in more physical terms if the isometry V is expressed via an

unitary operator U on $\mathcal{H}_A \otimes \mathcal{H}_B$ and a normalized vector $|\psi\rangle \in \mathcal{H}_B$ as

$$V|\phi\rangle = U|\phi\rangle \otimes |\psi\rangle.$$

Then, Eq. (1) becomes

$$\text{tr}_B U \rho_A \otimes \psi U^\dagger = \tau, \quad (2)$$

where ψ denotes the projection $|\psi\rangle\langle\psi|$. This relation might be interpreted within our thermalization scheme as follows: \mathcal{H}_B is the Hilbert space of a certain bath system B , ψ is its initial pure state, and U is the joint quantum-mechanical time-evolution of A and B .

Thus far, mathematical objects have been merely named with physical terms. The question is whether there is a \mathcal{T} representing isometry V such that the associated \mathcal{H}_B , U and ψ have a physically meaningful interpretation. A quite simple answer to that question is suggested if one looks at the dimensions d_A and d_B of the involved Hilbert spaces \mathcal{H}_A and \mathcal{H}_B . Assuming that d_A is finite, it is known that V can be realized as long as $d_B \geq d_A^2$. Hence, it is possible to find an isometry V for the choice $\mathcal{H}_B = \mathcal{H}_A \otimes \mathcal{H}_A$, which means that in this case the bath B can be thought to consist of just two copies A_1 and A_2 of the system $A_0 \equiv A$. This, in turn, suggests to choose the initial pure state $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_A$ as a purification of the thermal state τ of A_1 . I.e., for energy eigenstates $|0\rangle_1, |1\rangle_1, \dots, |d_A-1\rangle_1$ of A_1 with energies E_0, \dots, E_{d_A-1} , and for arbitrary orthogonal states $|0\rangle_2, |1\rangle_2, \dots, |d_A-1\rangle_2$ of A_2 let

$$|\psi\rangle = \frac{1}{Z} \sum_k e^{-\beta E_k} |k\rangle_1 \otimes |k\rangle_2, \quad (3)$$

which clearly satisfies $\text{tr}_{A_2} \psi = \tau$. As a consequence of this choice the joint unitary time evolution must be a product of a swap operation W on A_0 and A_1 ,

$$W|k\rangle_0 \otimes |k'\rangle_1 = |k'\rangle_0 \otimes |k\rangle_1, \quad (4)$$

and an arbitrary unitary operation U_2 on A_2 ,

$$U = W \otimes U_2. \quad (5)$$

The effect on A_0 in an arbitrary initial state ρ_A is

$$\begin{aligned} & \text{tr}_B (W \otimes U_2) \rho_A \otimes \psi (W \otimes U)^\dagger \\ &= \text{tr}_{A_1} W (\rho_A \otimes \text{tr}_{A_2} (\mathbf{1}_1 \otimes U_2) \psi (\mathbf{1}_1 \otimes U_2^\dagger)) W^\dagger \\ &= \text{tr}_{A_1} W (\rho_{A_1} \otimes \text{tr}_{A_2} \psi) W^\dagger \\ &= \text{tr}_{A_1} W (\rho_{A_1} \otimes \tau) W^\dagger \\ &= \text{tr}_{A_1} \tau \otimes \rho_A = \tau. \end{aligned}$$

This is the desired thermalization of A_0 .

For the remaining task of finding a physically meaningful Hamiltonian that generates the above dynamics we restrict ourselves to the simple case of system A_0 being a spin-1/2 in a magnetic field. It is a well-known fact that

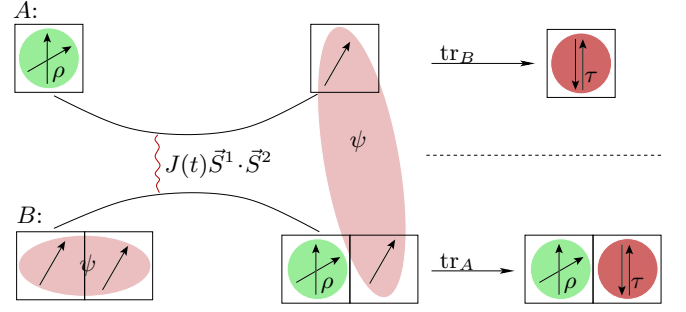


FIG. 1: A system spin (A) in an arbitrary initial state ρ interacts with two bath spins (B) in a pure, entangled initial state ψ . By the interaction the entanglement is swapped to the upper spin and the reduced state of the upper spin becomes a thermal state τ .

then the swap W can be generated by the Heisenberg-exchange interaction $\vec{S}^0 \cdot \vec{S}^1$ with an appropriate time-dependent coupling $J(t)$. [We use standard physics notation in units where $\hbar = 1$, i.e. $\vec{S} = (S_x, S_y, S_z) \equiv \frac{1}{2}(\sigma_1, \sigma_2, \sigma_3)$, $S_x^0 \equiv S_x^0 \otimes \mathbf{1}^1 \otimes \mathbf{1}^2$, etc.] In the end, this leads to a Hamiltonian

$$H(t) = \epsilon S_z^0 + \epsilon S_z^1 + J(t) \vec{S}^0 \cdot \vec{S}^1 + H_2, \quad (6)$$

where ϵ denotes the common spin-splitting energy for the spins A_0 and A_1 , and H_2 is an arbitrary Hamiltonian for the second bath spin A_2 . Making use of the identity $W = 2\vec{S}^0 \cdot \vec{S}^1 + \mathbf{1}/2$ it is straight forward to check that the time evolution $U = T_{\leftarrow} \exp -i \int_0^T H(t) dt$ generated by $H(t)$ over the time period $[0, T]$ can be written as

$$U = (\cos \alpha + iW \sin \alpha) \otimes U_2, \quad (7)$$

where the phase α is given by

$$\alpha = \frac{1}{2} \int_0^T J(t) dt, \quad (8)$$

and the unitary U_2 describes the time evolution of the second bath spin. Provided the time-dependent coupling $J(t)$ is such that the phase α is an odd multiple of $\pi/2$, the entire time evolution U is precisely of the form Eq. (5) that we aimed for.

The minimal thermalization model thus obtained is summarized in Fig. 1. It is worth emphasizing that the two bath spins in the pure state ψ together with the proposed interaction always lead to complete thermalization of the system spin, irrespective of the initial state ρ_A of the system spin. Also, the interaction is physical in the sense that it is a simple two-spin interaction; a three-spin interaction would comply with the mathematical formalism as well but is actually not required. Owing to the fact that the bath is microscopic its dynamics has to match the dynamics of the system to be thermalized. For this reason the spin-splitting energy of the system spin must equal the one of the first bath spin. In contrast to that, the local dynamics of the second bath

spin generated by H_2 does not change the entanglement with the two other spins and therefore is irrelevant for the thermalization. This offers a trivial interpretation of our model: Since the second bath spin is actually not involved in the system-bath interaction it can be traced out right from beginning. This leaves us with the first bath spin in the thermal state τ , which by the exchange interaction is then simply transferred to the system spin.

Another important point is that the coupling $J(t)$ has to be chosen such that the associated phase α must be an odd multiple of $\pi/2$. Here it is to mention that also in case of a macroscopic bath an interaction that is able to thermalize will have to obey conditions. For instance, a system-bath coupling that is instantaneously switched off will almost never leave the system in a thermal state. Yet, it seems to be clear that a macroscopic bath allows for more freedom in the choice of a thermalizing interaction. To illustrate the latter point we briefly discuss a simple generalization of the above minimal model.

The generalized model consists of a system spin A_0 and n pairs of bath spins denoted by $A_{\nu 1}$ and $A_{\nu 2}$ with $\nu = 1, \dots, n$. Initially, each spin pair $A_{\nu 1} A_{\nu 2}$ of the bath is in the kind of pure state Eq. (3) as in the minimal model. This defines an initial bath state ψ_n as a product of n entangled two-spin states, each being a purification of τ . Corresponding to the Hamiltonian of the minimal model, Eq. (6), the generalized model has the Hamiltonian

$$H = \epsilon S_z^0 + \epsilon \sum_{\nu=1}^n S_z^{\nu 1} + \sum_{\nu=1}^n J_\nu(t) \vec{S}^0 \cdot \vec{S}^{\nu 1} + \sum_{\nu=1}^n H^{\nu 2}.$$

The exchange interactions $\vec{S}^0 \cdot \vec{S}^{\nu 1}$ do not commute among each other. To allow for an analytical treatment we therefore assume that the couplings $J_1(t), \dots, J_n(t)$ are supported on disjoint time intervals $[0, t_1], [t_1, t_2], \dots, [t_n, T]$. With this assumption the time evolution operator on $A_0, A_{11}, \dots, A_{n1}$ can be written as the ordered product

$$\prod_{\nu}^{\leftarrow} (\cos \alpha_\nu + i W_{0\nu} \sin \alpha_\nu), \quad (9)$$

where $W_{0\nu}$ is the swap operation on $A_0, A_{\nu 1}$, and $\alpha_\nu = \frac{1}{2} \int_0^T J_\nu(t) dt$. The effect of the entire time evolution on the system spin A_0 can be easily computed if first all spins A_{12}, \dots, A_{n2} are traced out and then successively the partial traces over the bath spins $A_{11}, A_{21}, \dots, A_{n1}$ are taken. This is conveniently done by representing the density operators as matrices w.r.t. to the energy eigenstates $|0\rangle, |1\rangle$. In this way we find that an initial state of the system spin A_0

$$\rho_0 = \begin{pmatrix} a_{00} & a_{01} \\ a_{10} & a_{11} \end{pmatrix} \quad (10)$$

becomes a final state

$$\rho'_0 = \begin{pmatrix} p a_{00} & \lambda a_{01} \\ \lambda^* a_{10} & p a_{11} \end{pmatrix} + (1-p)\tau, \quad (11)$$

where τ is the thermal state, and the parameters p and λ are given by

$$p = \prod_{\nu=1}^n p_\nu, \quad \lambda = \prod_{\nu=1}^n \lambda_\nu,$$

with

$$p_\nu = \cos^2 \alpha_\nu, \\ \lambda_\nu = \cos^2 \alpha_\nu + i \cos \alpha_\nu \sin \alpha_\nu \tanh \frac{\beta \epsilon}{2}.$$

The moduli of p_ν and λ_ν are bounded above by unity, and they are less than unity as long as the phase α_ν is off an even multiple of $\pi/2$. For this reason, in the large n -limit generic interactions $J_\nu(t)$ will lead to very small parameters $p \ll 1$ and $|\lambda| \ll 1$, meaning that the final state is very close to the thermal state τ . This can be made more precise by stating that the trace distance of ρ'_0 to τ is upper bounded by $\sqrt{p^2 + |\lambda|^2}$. We conclude that the constraints that have to be imposed onto the couplings $J_\nu(t)$ in order to achieve thermalization are fairly weak in the generalized model.

Finally, a few remarks on entropy in the minimal model. Initially, the von Neumann entropy of the total system equals the entropy of system A , $S(\rho_A)$, because the initial pure state ψ of the bath has vanishing entropy. The unitary joint time evolution U leaves the total entropy unchanged, meaning that the final state $\rho'_{AB} = U \rho_A \otimes \psi U^\dagger$ of the joint system has also entropy $S(\rho_A)$. However, in the end the total system is “split” into system and bath. This means, by definition, that after the split system and bath can be accessed only by local observables of the form $O_A \otimes \mathbf{1}_B$ and $\mathbf{1}_A \otimes O_B$. With respect to these local observables the final state ρ'_{AB} is equivalent to a product state $\rho'_A \otimes \rho'_B$ [6], where the factors are the reduced states $\rho'_A = \text{tr}_B \rho'_{AB} \equiv \tau$ and $\rho'_B = \text{tr}_A \rho'_{AB} \equiv \rho_A \otimes U_2 \tau U_2^\dagger$. Hence, the final entropy of the split system in state $\rho'_A \otimes \rho'_B$ is $2S(\tau) + S(\rho_A)$, which exceeds the initial entropy by $2S(\tau)$. This entropy increase is precisely the entanglement entropy of the state ρ'_{AB} w.r.t. to A and B . In this way, the increase of the total entropy is seen to be the effect of the separation of the total system in system and bath.

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